DEPARTMENT OF PHYSICS, IIT MADRAS

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1. **Langevin description**. We begin by considering a single colloidal particle (a particle with size in microns) immersed in a thermally fluctuating fluid. The colloidal particle feels force from collisions with the fluid particles. The force that the colloidal particle feels has two parts: (i) systematic (deterministic) drag, which resists motion, and (ii) a stochastic (fluctuating) force, which has zero mean. The Langevin equation of motion of the colloidal sphere of mass m is then given as

$$m\frac{dV}{dt} = -\gamma V + F^P + \sqrt{2\gamma^2 D}\,\xi. \tag{1}$$

Here $\gamma = 6\pi\eta b$ is the friction of a sphere of radius b moving through a fluid of viscosity η, F^P is the net body force on the particle. The stochastic force ξ is zero mean and has no temporal correlations:

$$\langle\xi\rangle = 0, \qquad \langle\xi(t)\xi(t')\rangle = \delta(t-t') \tag{2}$$

The stochastic variable ξ is also called white noise as it has no correlation in time. Noises with temporal correlation are termed as colored noise. The choice of the constant $\sqrt{2\gamma^2 D}$ multiplying the stochastic variable ξ is for convenience, which will become clear after doing the following calculations.

(a) Why is the form of noise given in Eq.(2) a good model for experimentally measured trajectories of a colloidal particle in an aqueous medium?

(b) Using the above Langevin equation, show that:

$$\langle V(t)\rangle = V(0)e^{-\beta t}, \qquad \beta = \frac{\gamma}{m} \tag{3}$$

$$\langle V^2(t)\rangle = V_0^2 e^{-2\beta t} + D\beta\left(1 - e^{-2\beta t}\right) \tag{4}$$

(c) Using the equipartition theorem, show that the diffusion constant D must follow:

$$D = \mu_p\, k_B T = \frac{k_B T}{\gamma} = \frac{k_B T}{6\pi\eta b} \tag{5}$$

The above is called the Stokes-Einstein relation. It is an example of fluctuation-dissipation relation.

(d) Consider a dimensionless number $\mathrm{Re_p} = \rho_p U L/\eta$. Here ρ_p is the density of the particle, U is the typical speed, L is the typical length scale and η is the viscosity of the fluid. Using non-dimensionalisation, show that that Eq.(1) reduces to the overdamped Langevin equation, given below in Eq.(6), in the limit of $\mathrm{Re} \to 0$.

$$\frac{dx}{dt} = \mu_p\, F^P + \sqrt{2D}\,\xi = A + \sqrt{B}\,\xi. \tag{6}$$

(e) Derive the update equation for the above equation and show that it is:

$$x(t + \Delta t) = x(t) + \Delta t\, A + \sqrt{B\,\Delta t}\,\mathcal{N}(t). \tag{7}$$

Here $\mathcal{N}(t)$ is a Gaussian random variable with mean 0 and variance 1. The above is often called the Euler-Maruyama integrator.

(f) Defining $\Delta x(t) = x(t + \Delta t) - x(t)$, show that, to the leading order in Δt:

$$\langle \Delta x(t) \rangle = A\,\Delta t, \qquad \left\langle [\Delta x(t)]^2 \right\rangle = B\,\Delta t. \tag{8}$$

2. **Fokker-Planck description**. Show that the Fokker-Planck equation for the probability distribution $p(x, t)$, corresponding to the Langevin equation in (6) is:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(A\,p) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(B\,p) = -\frac{\partial J}{\partial x}. \tag{9}$$

3. **Brownian motion**. The simplest form of the Langevin equation in 1D is given as:

$$\frac{dx}{dt} = \sqrt{2D}\,\xi \tag{10}$$

The above describes the Brownian motion of a colloidal particle in 1D.

(a) Write the Euler-Maruyama integrator for the above.

(b) Solve the Fokker-Planck equation and obtain the PDF.

(c) What is the stationary PDF of a Brownian particle?

(d) Obtain the MSD (mean-squared displacement) of the Brownian particle, which is defined as

$$\mathrm{MSD}(t) = \langle [x(t + \tau) - x(\tau)]^2 \rangle = (2D)\,t \tag{11}$$

Here $\langle \ldots \rangle$ implies average over a long trajectory.

(e) The 1926 Nobel prize in physics was awarded to Perrin, among other things, to obtain the above MSD using experiments following a theoretical paper from Einstein [1]. Describe the theory paper and explain why was the verification of the Einstein's theory on Brownian motion a Nobel prize winning work.

4. **Ornstein-Uhlenbeck process** [2]. Consider a Brownian particle in 1D, which is confined in a harmonic potential (the resulting restoring force is $F^P = -kx$ [3]). The Langevin equation for the Ornstein-Uhlenbeck process is given as:

$$\frac{dx}{dt} = -\mu_p \, k \, x + \sqrt{2D}\,\xi = -\lambda \, x + \sqrt{2D}\,\xi \tag{12}$$

(a) Write the Euler-Maruyama integrator for the above.

(b) Obtain the stationary correlation function and its Fourier transform:

$$C(t - t') = \langle x(t)\, x(t') \rangle, \qquad C(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C(\Delta t)\, e^{-i\omega \Delta t}. \tag{13}$$

(c) Write the expression of the corresponding Fokker-Planck equation.

(d) Solve the Fokker-Planck equation to obtain the equilibrium PDF.

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[1] To quote from Einstein, Ann. Physik 322 (8): 549 (1905): *If the motion discussed here can actually be observed, then classical thermodynamics can no longer be looked upon as applicable with precision to bodies even of dimensions distinguishable in a microscope, and an exact determination of the actual atomic dimensions is then possible.*

[2] OUP is the only continuous stochastic process that is simultaneously stationary, Gaussian, and Markovian. See the paper titled 'The Brownian Movement and Stochastic Equations' by JL Doob (1942).

[3] A harmonic confinement of a colloidal particle is possible using optical tweezers, whose discoverer - Arthur Ashkin - was awarded the Nobel prize in Physics (2018) for the discovery [4].

[4] A. Ashkin, Nobel lecture: Optical tweezers and their application to biological systems (2018).